1,6-Bis(4-chlorophenyl)-8-(4-pyridyl)-3,4-dihydro-pyrrolo[1,2-a]pyrazine

Xiao-Yang Qiu,[a,b] Wei-Sheng Liu,[b]* Hai-Liang Zhu[c]* and Ji-Long Ma[a]

[a]Department of Chemistry, Fuyang Normal College, Fuyang Anhui 236041, People's Republic of China, [b]Department of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China, and [c]Institute of Functional Biomolecules, State Key Laboratory of Pharmaceutical Biotechnology, Nanjing University, Nanjing 210093, People's Republic of China

Correspondence e-mail: liuws@lzu.edu.cn, hailiang_zhu@163.com

Key indicators

Single-crystal X-ray study

$T = 298$ K

Mean σ(C–C) = 0.006 Å

R factor = 0.076

wR factor = 0.174

Data-to-parameter ratio = 13.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the crystal struture of the title compound, $C_{24}H_{17}Cl_2N_3$, the two benzene rings and the pyridyl group lie in a propeller arrangement around the central ring system, thereby minimizing steric effects among these rings.

Comment

As part of the structural characterization of multi-ring compounds, we report here the structure of the title compound, (I).

(I)
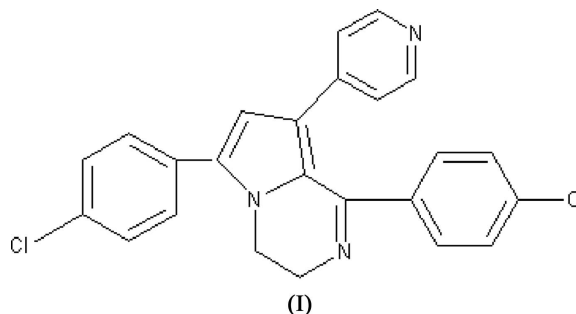
In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C16═N3 bond length of 1.290 (5) Å conforms to the value for a double bond. The bond lengths of 1.372 (5) and 1.387 (5) Å for C7═C8 and C9═C10 are greater than that for a double bond and less than the value for a single bond because of conjugation effects in the molecule. The two benzene rings and the pyridyl group lie in a propeller arrangement around the central ring system, thereby minimizing steric effects among these rings. The pyrazine ring adopts a sofa conformation, with C23 displaced by 0.62 (4) Å from the plane of the other five atoms. The dihedral angle between the planes of the pyridyl and pyrrole rings is 41.9 (5)°. Benzene rings C1–C6 and C17–C22 form dihedral angles of 35.2 (5) and 58.3 (5)°, respectively, with the pyrrole ring.
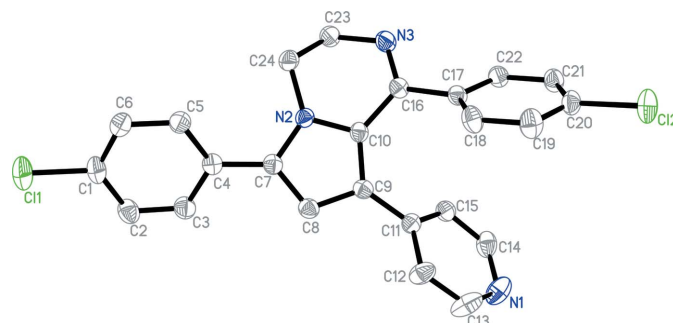
Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted.

organic papers

Experimental

The title compound was synthesized by the reaction of equivalent amounts of (E)-1-(4-chlorophenyl)-3-(4-pyridyl)prop-2-en-1-one, 1,2-diaminoethanone and 1-(4-chlorophenyl)ethanone in an ethanol solution for 8 h at 373–383 K. Single crystals suitable for X-ray diffraction analysis were obtained by evaporation of an acetone solution.

Crystal data

$C_{24}H_{17}Cl_2N_3$	$D_x = 1.371$ Mg m^{-3}
$M_r = 418.31$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2865
$a = 10.450 (2)$ Å	reflections
$b = 10.495 (2)$ Å	$\theta = 5.0–12.5°$
$c = 18.938 (4)$ Å	$\mu = 0.34$ mm^{-1}
$\beta = 102.73 (3)°$	$T = 298 (2)$ K
$V = 2026.0 (7)$ Å^3	Block, brown
$Z = 4$	$0.42 \times 0.15 \times 0.07$ mm

Data collection

Bruker SMART APEX area-detector diffractometer	3553 independent reflections
	2670 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.043$
Absorption correction: multi-scan	$\theta_{max} = 25.0°$
(SADABS; Sheldrick, 1996)	$h = -12 \rightarrow 12$
$T_{min} = 0.935$, $T_{max} = 0.967$	$k = -12 \rightarrow 12$
8122 measured reflections	$l = -15 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0608P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.077$	$+ 1.6146P]$
$wR(F^2) = 0.174$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.027$
3553 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
262 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C7—C8	1.372 (5)	C14—N1	1.324 (6)
C7—N2	1.379 (4)	C16—N3	1.290 (5)
C9—C10	1.387 (5)	C23—N3	1.458 (5)
C10—N2	1.370 (4)	C24—N2	1.459 (5)
C11—C12	1.385 (5)		
C8—C9—C10—C16	174.7 (4)	C16—C10—N2—C24	5.5 (5)
N3—C16—C17—C22	−43.4 (5)	C8—C7—N2—C24	177.9 (4)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å. and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). J. Chem. Soc. Perkin Trans. 2, pp. S1–19.
Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Winconsin, USA.
Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
Sheldrick, G. M. (1997b). SHELXS97. Version 5.1. AXS Inc., Madison, Wisconsin, USA.